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(NASA-CR-169941) LABORATORY STUDIES AT HIGH
RESOLUTION OF THE INFRARED ABSORPTION
SPECTRA OF A NUMBER OF GASES FOUND IN
PLANETARY ATMOSPHERES Final Report (Florida
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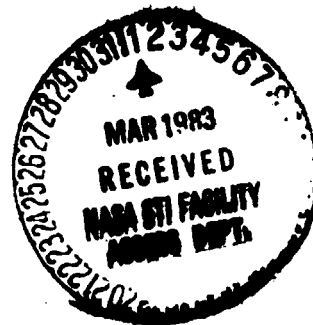
Final Report

NASA Grant NGR 10-004-056

Department of Physics

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I. Background

The work funded for the past 14 years under NASA Grant NGR 10-004-056 has been concerned with laboratory studies at high resolution of the infrared absorption spectra of a number of gases found in planetary atmospheres. The primary objective of such studies is to provide absorption line measurements which can be of value for the interpretation of planetary spectra in terms of molecular abundances and conditions in the planetary atmospheres.

The high resolution spectra taken in this work have yielded measurements of individual vibration-rotation line parameters including positions, strengths, pressure broadened widths and, where assignments were unknown, the temperature sensitivity of the strengths. Such information allows the determinations of the absorption of a given molecular gas under planetary conditions of temperature and pressure and at the same time it provides the data necessary if the spectra are to be understood in terms of basic molecular theory. Thus this work has included spectral analysis in the form of line assignments as well as fitting of the data to Hamiltonian models. Such fitting is very useful in that it helps to confirm and extend the assignments. This approach has been particularly valuable for interpreting the infrared spectrum of methane as this spectrum is composed of many closely spaced lines often of quite different temperature sensitivity.

II Laboratory Facilities

The primary source of the spectra analyzed for this project was the four-pass grating spectrometer located in the Physics department at The Florida State University. Most of the studies were performed at wavelengths between 1.5 and 4 microns with a resolution of 0.02 cm^{-1} . A limited amount of work

was done between 0.6 and 1.1 microns at a resolution of about 0.1 cm^{-1} .

During the past three years some supplementary spectra were obtained at 0.01 cm^{-1} resolution with the Fourier transform instrument located in the Solar telescope laboratory at the Kitt Peak Observatory. Because of the superior resolution and wavenumber determination possible with a high quality instrument of this type, it was decided two years ago to begin the construction of a 0.0025 cm^{-1} resolution Fourier instrument in our own laboratory. It is expected that this instrument will be operational during the present calendar year.

A wide variety of absorption cells were constructed for the grant studies. One of the most useful was a 5 meter base length White-type cell coolable to a temperature of about 120 K. This was used in several methane studies.

III Results

Details of the research performed with the aid of funding by this grant may be found by consulting the various publications listed subsequently in this report. The following is a brief summary of the purpose, nature, and scope of the major projects undertaken.

- 1) The initial work performed under this grant was a study of the temperature dependence of the strengths of methane absorption lines near 8400 \AA . This information was desired for comparison with ground based Jovian spectra. With a 160 meter path in the White cell, it was determined that most of the features observed in the lab did not show strong relative changes in intensity with temperature. These results were sent to Dr. Carleton of The Smithsonian Observatory for comparison with his spectra.
- 2) Following the work above, extensive measurements were made on the line intensities of CO_2 . More than a thousand lines belonging to a total of 18 different

bands were measured in the region from 7000 to 3000 cm^{-1} . The results were analyzed for the effects of Coriolis and Fermi interactions and considerable progress was made in obtaining a theoretical calculation of relative line intensities.

3) Following the CO_2 studies, a concerted effort was begun to understand the spectrum of methane between 4500 and 2500 cm^{-1} . The results obtained over a seven year period in collaboration with several other laboratories were very satisfying. Between 3250 and 2500 cm^{-1} , over 8000 absorption lines were assigned to some 10 absorption bands of $^{12}\text{CH}_4$ and $^{13}\text{CH}_4$. This represents almost every line of consequential intensity in this region. In addition the strength of each line was also measured and the results catalogued on the AFGI tape. In the 4500 to 4100 cm^{-1} region new assignments for the $\nu_3 + \nu_4$ band were obtained.

The results of the above study also had an important bearing on the ν_2 , ν_4 fundamental region near 1600 cm^{-1} . Using the results of our study, other workers were then able to determine the "hot-band" lines in this latter region.

4) During the past two years we have been engaged in a major construction project to replace our grating spectrometer with a Fourier transform spectrometer capable of a factor of ten improvement in resolution and wavenumber accuracy. This instrument should become operational this year. With it we plan to examine some of the heavier molecular species in addition to broadening our region of coverage of the lighter ones.

IV. Papers published on work partially supported
by this Grant

1. Line Intensities of $C^{13}O_2^{16}$ in the 1.43 to 1.65 Micron Region, R. A. Toth, R. H. Hunt, and E. K. Plyler, J. Mol. Spectry. 38, 107 (1971).
2. Measurement and Analysis of the ν_3 Band of CH_4 , William L. Barnes, Joel Susskind, Robert H. Hunt and E. K. Plyler, J. Chem. Phys. 56, 5160, (1972).
3. Line Intensities of CO_2 in the 2.0 Micron Region, H. D. Downing and R. H. Hunt, J. Quant. Spectry. and Radiative Transfer 13, 311 (1973).
4. Line Intensities of CO_2 in the 2.7 Micron Region, H. D. Downing, L. R. Brown and R. H. Hunt, J. Quant. Spectry. and Radiative Transfer 15, 205 (1975).
5. Coriolis intensity Perturbations in π - Σ Bands of CO_2 , H. D. Downing, B. J. Krohn and R. H. Hunt, J. Mol. Spectros. 55, 66 (1975).
6. Analysis of the OH Stretching Band of Methanol, R. G. Lee, R. H. Hunt, E. K. Plyler and D. M. Dennison, J. Mol. Spectrosc. 57, 138 (1975).
7. Line Intensities and Strengths of Methane in the $2862-3000\text{ cm}^{-1}$ Region, R. A. Toth, L. R. Brown, and R. H. Hunt, J. Mol. Spectrosc. 67, 1 (1977).
8. Line Intensities of Methane in the $2700-2862\text{ cm}^{-1}$ Region, R. H. Hunt, L. R. Brown and R. A. Toth, J. Mol. Spectrosc., 69, 482 (1978).
9. The Ground State of H_2CO , L. R. Brown, and R. H. Hunt, J. Mol. Spectrosc. 73, 277 (1978).
10. Frequencies, Line strengths, and Assignments in the Doppler-Limited Spectrum of Formaldehyde from $2700-3000\text{ cm}^{-1}$, L. R. Brown, R. H. Hunt and A. S. Pine, J. Mol. Spectrosc. 75, 406 (1979).

11. Torsion-Rotation Levels of the OH-Stretch Fundamental of CD_3OH , David G. Snyder and Robert H. Hunt J. Mol. Spectrosc. 78, 422 (1979).
12. Line Intensities, Spin Splittings and Frequencies in the $\nu_1 + \nu_3$ Band of NO_2 , R. A. Toth and R. H. Hunt, J. Mol. Spectrosc. 79, 182 (1980).
13. Extended Line Assignments for the $\nu_3 + \nu_4$ Band of $^{12}\text{CH}_4$, R. H. Hunt, L. R. Brown, R. A. Toth and J. W. Brault, J. Mol. Spectrosc. 86, 159-169 (1981).
14. Line Assignments and Intensities for the $\nu_3 + \nu_4 + \nu_4$ Band of $^{12}\text{CH}_4$, R. H. Hunt, L. R. Brown, R. A. Toth and J. W. Brault, J. Mol. Spectrosc. 86 170-183 (1981).
15. Absorption Line Parameters for Methane from 2385 to 3200 cm^{-1} , R. A. Toth, L. R. Brown, R. H. Hunt and L. S. Rothman Appl. Opt. 20, 932-935 (1981).
16. Line Assignments and Intensities for the $\nu_3 + \nu_2 - \nu_2$ Band of $^{12}\text{CH}_4$, L. R. Brown, R. A. Toth, R. H. Hunt and J. W. Brault, J. Mol. Spectrosc. 89, 528-541 (1981).
17. Molecular Constants for the Interacting Upper States of the $\nu_1, \nu_3, 2\nu_2, \nu_2 + \nu_4$ and $2\nu_4$ Band in $^{12}\text{CH}_4$, J. E. Lolck, A. G. Robiette, L. R. Brown, and R. H. Hunt, J. Mol. Spectrosc. 92 229-245 1982.
18. Measurement and Analysis of the Infrared Absorption Spectrum of the $2\nu_2$ Band of $^{12}\text{CH}_4$, R. H. Hunt, L. R. Brown, J. E. Lolck and A. G. Robiette, J. Mol. Spectrosc. 92, 246-256 (1982).

V. Financial position

All grant funds have been expended.